To appear at Conference on Decision and Control (CDC), 2021

# Robustness Guarantees for Structured Model Reduction of Dynamical Systems

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***Abstract*— Model reduction methods usually focus on the error performance analysis; however, in presence of uncertainties, it is important to analyze the robustness properties of the error in model reduction as well. In this paper, we give robustness guarantees for structured model reduction of linear and nonlinear dynamical systems under parametric uncertainties. In particular, we consider a model reduction where the states in the reduced model are a strict subset of the states of the full model, and the dynamics for all other states are collapsed to zero (similar to quasi-steady state approximation). We show two approaches to compute a robustness metric for any such model reduction — a direct linear analysis method for linear dynamics and a sensitivity analysis based approach that also works for nonlinear dynamics. We also prove that for linear systems, both methods give equivalent results.**

## I. Introduction

For applications of control theory to physical system design, a reduced model is commonly used that describes the dynamics of interest in lower dimensions to simplify the design process. A common way to obtain a reduced model from a detailed model of a system is to make use of different time scales in the full system dynamics. Singular perturbation theory [1] is the formal way of deriving reduced models for system dynamics with time-scale separation. A key feature of singular perturbation theory is that the states of the reduced model are a subset of the states of the full model. In other words, the structure of the model and the meaning of the states and parameters is conserved by construction in any reduced model obtained using singular perturbation theory. This is not automatically the case in other model reduction techniques where transformations are introduced [2] [3] and hence in such techniques, the meanings of the states may not be preserved. We define structured model reduction in this paper as the set of model reduction methods where the states of the reduced models are a strict subset of the states of the full model.

The advantage of structured model reduction techniques is that an explicit mapping between the full and the reduced model is readily available [4]. Moreover, since the parameters and the states in the reduced model have the same meaning as in the full model, the design outputs and analysis results obtained using the reduced model can easily be given context and compared with the full model [5]. Due to the strict condition on the possible reduced model states, the structured model reduction methods suffer from the limitation that the choice of reduced models is limited and dependent on the modeling details of the full system. In other words, for a given full model it may not always be possible to analytically derive a reduced model. Other model reduction methods that are projection-based or those which preserve the input-output mapping are better in that respect [6], [7]. In this paper, we focus on the former class of model reduction problems that preserve the modeling structure in the reduced models.

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The goal with any model reduction problem is to minimize the error in the performance of the reduced model when compared to the full model. This error performance criterion can be general and depend on trajectories of all states and output variables, or specific, such as minimizing a particular metric of interest. Singular perturbation theory for model reduction and its error analysis is a widely studied topic in the literature for different system and control design settings [8]–[10]. A commonly used method for model reduction that is derived from the singular perturbation concept of time-scale separation is the quasi-steady state approximation method (QSSA) [11]–[14]. Here, a subset of states is assumed to be at steady-state and hence their dynamics are collapsed to algebraic relationships. Error analysis for QSSA based model reduction has been studied in [15]–[17]. However, robustness of these model reduction methods is not widely studied in the literature.

Robust control design is a well-studied problem in control theory. The extensions of robust control theory to singularly-perturbed systems have been studied in [18] and [19]. Similarly, robust stability analysis of adaptive control problems, linear time-varying systems, and the general parametric uncertainty problems has been of interest as well [20] [21]. A complementary, although not as widely applicable, approach to study the robustness of systems is to use sensitivity analysis of system variables or derived properties under parameter variations. Due to the success of robust control design methods [20] for different applications, the more holistic approach of sensitivity analysis for robustness estimates has not received much attention. In [22], sensitivities of singular values are used to give estimates for robustness properties of a linear feedback system. The advantage of such a method is that it can be used to analyze the effect of multiple parametric uncertainties and hence can be used to enhance the usual robust stability approaches.

Our problem statement is motivated by this sensitivity analysis approach for robustness and by the lack of existing results for robustness estimates of error in structured model reduction. In particular, we give robustness guarantees for the error in model reduction under parametric uncertainties. Using linear analysis, we give a robustness metric for QSSA-style model reduction of linear dynamical systems. We present a complementary approach that employs sensitivity analysis of the error in model reduction to estimate the robustness under parametric uncertainties. This approach works for nonlinear dynamical systems as well. Finally, we compare these results and show examples to numerically demonstrate our findings.

## II. Preliminaries

### A. Notation

We denote an eigenvalue of a matrix $P$ by $\lambda(P)$. The maximum eigenvalue will be denoted by $\lambda_{\max}(P)$. For a state-dependent matrix $P(x)$ we denote the maximum eigenvalue of $P$ over all values of $x$ by $\lambda_{\max_x}(P)$. Throughout this paper, we consider the Euclidean 2-norm for vectors with the notation $\|x\|$ for the 2-norm of $x \in \mathbb{R}^n$ and similarly for matrices $\|\cdot\|$ represents the induced 2-norm.

### B. Problem Formulation

The full system model is given by the following linear autonomous state-space equation

$$\dot{x} = A(\theta)x, \quad y = Cx, \quad x(0) = x_0, \tag{1}$$

where $x \in \mathbb{R}^n$ are state variables, the output vector is $y \in \mathbb{R}^k$ and $\theta = \left[\theta_1, \theta_2, ..., \theta_p\right]^T$ is the vector of all model parameters. We consider a structured model reduction in this paper where the dynamics of a subset of states ($x_c$) are collapsed (converted to algebraic relationships) on account of being at quasi-steady state. The remaining states are the states of the reduced model, $\hat{x}$. The reduced model is given by

$$\dot{\hat{x}} = \hat{A}(\theta)\hat{x}, \quad \hat{y} = \hat{C}\hat{x}, \quad \hat{x}(0) = \hat{x}_0, \tag{2}$$

where $\hat{x} \in \mathbb{R}^{\hat{n}}$ are the reduced state variables and $\hat{y} \in \mathbb{R}^k$ is the output vector. We assume that the full and the reduced model have the same number of outputs but different dynamics. Throughout this paper, we also assume that both the full and the reduced systems are asymptotically stable and observable. This model reduction is a relaxed form of singular perturbation theory based model reduction in that it does not require the system to be in the standard separable form, which is a hard condition to satisfy for general system dynamics, as we will see next.

Singular perturbation theory [1] is the standard way

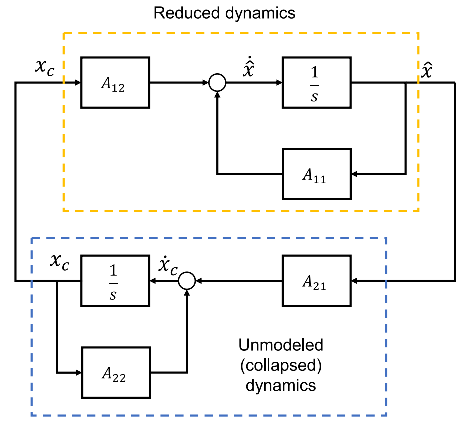


Fig. 1. Structured model reduction of a linear system. The $1/s$ block represents an integrator.

to derive reduced models and bounds on error in model reduction for the problem statement given above. However, to use singular perturbation theory the system dynamics need to be separable according to the different time-scales. For the problem formulation above, the requirement would be that we can write the dynamics in the following form,

$$\begin{aligned} \dot{\hat{x}} &= A_{11}\hat{x} + A_{12}x_c, \\ \epsilon\dot{x}_c &= A_{21}\hat{x} + A_{22}x_c, \end{aligned} \tag{3}$$

where $A_{11} \in \mathbb{R}^{\hat{n}\times\hat{n}}$, $A_{22} \in \mathbb{R}^{(n-\hat{n})\times(n-\hat{n})}$, and similarly we have $A_{12}$ and $A_{21}$. Now, under the condition that the time scale separation parameter $\epsilon \to 0$ and Hurwitz $A_{22}$, we get the reduced model as in equation (2) with,

$$\dot{\hat{x}} = (A_{11} - A_{12}A_{22}^{-1}A_{21})\hat{x} := \hat{A}\hat{x}. \tag{4}$$

In Figure 1, the block diagram for a system with time-scale separation is given. Using singular perturbation theory, conditions can be derived under which the error in model reduction converges to zero:

$$\|x - \hat{x}\| \leq O(\epsilon) \tag{5}$$

for $\epsilon \in [0, \epsilon^*]$. The error in model reduction goes to zero as $\epsilon \to 0$. This is the standard model reduction problem using singular perturbation to separate the time-scales of the model where the dynamics of the "fast" states of the system ($x_c$) are collapsed to zero when $\epsilon \to 0$ and the dynamics of the "slow" states ($\hat{x}$) is the reduced dynamics.

Under uncertainties in the system dynamics, it is important to analyze the robustness of the model reduction. The results on robustness for singular perturbation based model reduction either focus on robust controller design under uncertainties for singularly perturbed systems [18] [19] or analyze the effect on the time-scale separation parameter $\epsilon$ due to uncertainties. Recently, a singular perturbation margin [23] (similar to the gain margin and phase margin definitions) has been proposed to assess the robust stability of singularly perturbed systems under uncertainties. It is defined using the $\epsilon^*$ given in the error approximation equation (5). This framework can be used to compute a robustness estimate of the model reduction error for singular perturbation method. An extension of this robust stability margin for nonlinear dynamics is given in [24]. Despite the rich body of literature on singular perturbation theory, the major limitation of such a model reduction approach remains that the system dynamics must be written in the standard form (3). As stated in [25], for physical systems it is usually not straightforward to put a model in the singularly perturbed form since the choice of combination(s) of parameters to be considered small is not always clear. Hence, the relaxed approach of using QSSA is common for various applications.

In QSSA, the dynamics of a set of states are collapsed to zero to get the reduced-order model. The choice of states to be collapsed is usually driven by known time-scale separations in the system model. Although QSSA is a widely used approach it does not necessarily guarantee error performance as in equation (5). The limitation of QSSA is that the mathematical justification and conditions for approximating a variable to be at steady state are not always obvious. As a result, there could be many possibilities of reduced models and so it is the designer's task to find a "correct" QSSA based model reduction. Towards that end, in [17], a structured model reduction algorithm is presented that guides the choice of collapsed states so that the error between the output of the full and the reduced models is minimized. Other QSSA error analysis [15], [26] approaches can also be used for this purpose. In this paper, we study the problem of robustness of this structured model reduction, that is, how robust a particular model reduction is under parametric uncertainties.

To formulate this problem, we first construct an augmented state-space system that consists of variables of the full model as well as the reduced model:

$$\bar{x} := \begin{bmatrix} x \\ \hat{x} \end{bmatrix}.$$

We denote all augmented variables similarly with a bar on top of the usual variables. So,

$$\bar{A} := \begin{bmatrix} A & 0 \\ 0 & \hat{A} \end{bmatrix}.$$

For the augmented state variable, we can write the following state-space system,

$$\dot{\bar{x}} = \bar{A}(\theta)\bar{x}, \quad \zeta = \bar{C}\bar{x}, \qquad \bar{x}(0) = \begin{bmatrix} x_0 \\ \hat{x}_0 \end{bmatrix}, \tag{6}$$

where $\zeta$ is the error in model reduction defined as $\zeta = y - \hat{y}$, hence $\bar{C} = \begin{bmatrix} C & -\hat{C} \end{bmatrix}$. To study the robustness of the structured model reduction (that is the robustness of deriving the particular reduced model $(\hat{x}, \hat{A})$ with respect to uncertainties in model parameters) we need an upper bound on $\|\zeta\|$ as the parameters $\theta$ vary. For the linear augmented system we can write the following by solving for $\zeta(t, \theta)$,

$$\zeta(t, \theta) = \bar{C} e^{\bar{A}t} \bar{x}(0), \tag{7}$$

where $\zeta \in \mathbb{R}^k$.

**Lemma 1** (See [27])**.** *For a Hurwitz matrix $A$, the norm of the matrix exponential is bounded above as*

$$\left\| e^{At} \right\| \leq e^{-|\mu| t},$$

*where $\mu$ is the logarithm norm of $A$ [28]. For the log-norm induced by the 2-norm, we have that*

$$\mu(A) = \frac{\lambda_{\max}(A + A^T)}{2},$$

*and for Hurwitz $A$, $\mu$ is always negative.*

We use this to give an important result on the derivative of the matrix exponential with respect to a parameter.

**Lemma 2.** *The derivative of the matrix exponential $e^{At}$ with respect to a parameter $\theta_i$ is given by*

$$\frac{\partial e^{At}}{\partial \theta_i} = \int_0^t e^{(t-\tau)A} \frac{\partial A}{\partial \theta_i} e^{\tau A} d\tau. \tag{8}$$

*If $A$ is Hurwitz, the norm of the derivative of the matrix exponential with $\theta_i$ is bounded above by*

$$\left\| \frac{\partial e^{At}}{\partial \theta_i} \right\| \leq \left\| \frac{\partial A}{\partial \theta_i} \right\| t e^{-|\mu| t}. \tag{9}$$

*where $|\mu|$ is the absolute value of the log-norm of $A$ as in Lemma 1.*

*Proof.* The first part of the lemma (in equation (8)) is a result proven in [29] and a simplified version is given in [30] and [31]. We give an alternative proof in the Appendix. To prove the second part, given in equation (9), write the norm of the derivative of the matrix exponential with respect to a parameter $\theta_i$ as

$$\begin{aligned} \left\| \frac{\partial e^{At}}{\partial \theta_i} \right\| &= \left\| \int_0^t e^{(t-\tau)A} \frac{\partial A}{\partial \theta_i} e^{\tau A} d\tau \right\| \\ &\leq \int_0^t \left\| e^{(t-\tau)A} \right\| \left\| \frac{\partial A}{\partial \theta_i} \right\| \left\| e^{\tau A} \right\| d\tau. \end{aligned}$$

Now using the result of Lemma 1, since $A$ is Hurwitz, we have,

$$\left\| \frac{\partial e^{At}}{\partial \theta_i} \right\| \leq \left\| \frac{\partial A}{\partial \theta_i} \right\| \int_0^t e^{-(t-\tau)|\mu|} e^{-\tau|\mu|} d\tau.$$

Solving the above integral, we get the desired result:

$$\left\| \frac{\partial e^{At}}{\partial \theta_i} \right\| \leq \left\| \frac{\partial A}{\partial \theta_i} \right\| t e^{-|\mu| t}. \qquad \square$$

With the result from Lemma 1, we can conclude that under our assumption of asymptotically stable full and reduced models, we have that $\bar{A}$ is Hurwitz, and hence the error dynamics given in equation (7) converges to zero at steady-state. In this way, we have set up the problem to focus solely on the analysis of the robustness of model reduction while assuming that the important problem of minimizing the model reduction error has already been addressed. For a given structured model reduction (and hence the corresponding augmented system above), we can get a bound on the error in model reduction as the model parameters vary to give a robustness estimate for this model reduction. We construct a normalized [32] robustness distance estimate, $d_R$, for this purpose by computing the change in error with parameter perturbations around any nominal values given by $\theta_i^*$:

$$d_R = \sum_{i=1}^{p} \frac{\theta_i^*}{\|\zeta(t,\theta_i^*)\|} \cdot \left\| \frac{\partial \zeta}{\partial \theta_i}\bigg|_{\theta_i=\theta_i^*} \right\|, \tag{10}$$

where $\zeta(t,\theta_i^*)$ is the non-zero error in model reduction for $t > 0$ and parameter $\theta_i = \theta_i^*$. Using $d_R$, we propose a robustness metric to determine the performance of reduced models under parameter uncertainties:

$$R = \frac{1}{1+d_R} = \frac{1}{1+\sum_{i=1}^{p} \frac{\theta_i^* \left\| \frac{\partial \zeta}{\partial \theta_i}\big|_{\theta_i=\theta_i^*} \right\|}{\|\zeta(t,\theta_i^*)\|}}. \tag{11}$$

We define the sensitivity of the error with respect to a parameter $\theta_i$ in the equation above as $S_\zeta$:

$$S_\zeta = \frac{\partial \zeta}{\partial \theta_i},$$

where $S_\zeta \in \mathbb{R}^k$. Hence, our goal in this paper is to compute $R$ to give robustness estimate under parametric uncertainties when reducing a dynamical model. Towards that end, we derive bounds on $\|S_\zeta\|$ that can then be used to compute an overall robustness metric using equation (11).

## III. Results

### A. Linear System — Uncertain Initial Conditions

In this section, we consider the uncertainties in the initial conditions — $x(0)$ of a linear system. We can use this result to assess the robust performance of different possible structured model reductions when the initial conditions are dependent on the uncertain model parameters.

**Theorem 1.** *For the structured model reduction of the autonomous linear system (1) to the reduced form of system (2) by using time-scale separation and quasi-steady state approximation under uncertain initial conditions, the norm of the sensitivity of the error in model reduction $S_\zeta$ is bounded above by*

$$\|S_\zeta\|_2^2 \leq \lambda_{\max}(P) \left\| \frac{\partial \bar{x}(0)}{\partial \theta_i} \right\|_2^2,$$

*where $P$ is the Lyapunov matrix that solves the equation $\bar{A}^T P + P\bar{A} = -\bar{C}^T\bar{C}$.*

*Proof.* We have the 2-norm [20] of $S_\zeta$ defined as:

$$\|S_\zeta\|_2^2 = \int_0^\infty S_\zeta(t)^T S_\zeta(t) dt.$$

Using equation (7), we can write $S_\zeta$ for a parameter $\theta_i$ as,

$$S_\zeta = \bar{C} e^{\bar{A}t} \frac{\partial \bar{x}(0)}{\partial \theta_i},$$

since we have assumed that the matrices $\bar{A}$ and $\bar{C}$ are not dependent on parameters. The norm of $S_\zeta$ then becomes

$$\|S_\zeta\|_2^2 = \int_0^\infty \left(\frac{\partial \bar{x}(0)}{\partial \theta_i}\right)^T e^{\bar{A}^T t} \bar{C}^T \bar{C} e^{\bar{A}t} \left(\frac{\partial \bar{x}(0)}{\partial \theta_i}\right) dt. \tag{12}$$

From [33, Ch.5], we know that for an asymptotically stable system, there exists a unique matrix $P$ that solves the Lyapunov equation $\bar{A}^T P + P\bar{A} = -\bar{C}^T\bar{C}$ given by the observability Gramian:

$$P = \lim_{N\to\infty} W_{\mathrm{o}}(N) = \lim_{N\to\infty} \int_0^N e^{\bar{A}^T t} \bar{C}^T \bar{C} e^{\bar{A}t} dt,$$

where $W_{\mathrm{o}}(N)$ is the observability Gramian. Substituting this into equation (12) gives us the desired result:

$$\|S_\zeta\|_2^2 = \left(\frac{\partial \bar{x}(0)}{\partial \theta_i}\right)^T \left[\int_0^\infty e^{\bar{A}^T t} \bar{C}^T \bar{C} e^{\bar{A}t} dt\right] \left(\frac{\partial \bar{x}(0)}{\partial \theta_i}\right)$$

$$\Rightarrow \|S_\zeta\|_2^2 \leq \lambda_{\max}(P) \left\| \frac{\partial \bar{x}(0)}{\partial \theta_i} \right\|_2^2. \qquad \square$$

### B. Linear System — Uncertain System Dynamics

Now we consider the case where the system dynamics given by the $\bar{A}(\theta)$ matrix is dependent on uncertain parameters. For simplicity we denote $\bar{A}(\theta) := \bar{A}$, noting that it is parameter-dependent.

**Theorem 2.** *For the structured model reduction of the autonomous linear system (1) to the reduced form of system (2) by using time-scale separation and quasi-steady state approximation under uncertain system dynamics, the norm of the sensitivity of the error in model reduction $S_\zeta$ is bounded above by*

$$\|S_\zeta\|_2^2 \leq \tilde{M} \left\| \frac{\partial \bar{A}}{\partial \theta_i} \right\|_2^2 \left\|\bar{C}^T\bar{C}\right\|_2 \|\bar{x}(0)\|_2^2,$$

*where $\tilde{M} = 1/(4|\mu|^3)$ and $\mu$ is dependent on $\bar{A}$ as given in Lemma 1.*

*Proof.* Write the norm of $S_\zeta$ as

$$\|S_\zeta\|_2^2 = \int_0^\infty S_\zeta(t)^T S_\zeta(t) dt. \tag{13}$$

To derive the bounds, we first write the partial derivative of $\zeta(t,\theta)$ with respect to a parameter $\theta_i$ as given in equation (7),

$$S_\zeta = \frac{\partial \zeta}{\partial \theta_i} = \bar{C} \frac{\partial e^{\bar{A}t}}{\partial \theta_i} \bar{x}(0), \tag{14}$$

assuming that the output matrix $\bar{C}$ and the initial conditions are independent of model parameters. We can write the norm of $S_\zeta$ as,

$$\|S_\zeta\|^2 = \int_0^\infty \bar{x}(0)^T \left(\frac{\partial e^{\bar{A}t}}{\partial \theta_i}\right)^T \bar{C}^T\bar{C} \left(\frac{\partial e^{\bar{A}t}}{\partial \theta_i}\right) \bar{x}(0)dt,$$
$$\leq \int_0^\infty \left\|\frac{\partial e^{\bar{A}t}}{\partial \theta_i}\right\|^2 \left\|\bar{C}^T\bar{C}\right\| \|\bar{x}(0)\|^2 \, dt.$$

Using the result from Lemma 2, we can write,

$$\|S_\zeta\|^2 \leq \left\|\frac{\partial \bar{A}}{\partial \theta_i}\right\|^2 \left\|\bar{C}^T\bar{C}\right\| \|\bar{x}(0)\|^2 \int_0^\infty t^2 e^{-2|\mu|t} dt.$$

We can evaluate the integral above by parts:

$$\int_0^\infty t^2 e^{-2|\mu|t} dt = \frac{1}{4\,|\mu|^3}.$$

We get the desired result for the norm of $S_\zeta$ by substituting this integral,

$$\|S_\zeta\|^2 \leq \frac{1}{4\,|\mu|^3} \left\|\frac{\partial \bar{A}}{\partial \theta_i}\right\|^2 \left\|\bar{C}^T\bar{C}\right\| \|\bar{x}(0)\|^2 .$$

The robustness estimate $R$ follows by using the above bound and equation (11). □

**Corollary 2.1.** *Under simultaneous parametric uncertainties in system dynamics and initial conditions, we can write the norm of $S_\zeta$ as*

$$\|S_\zeta\|_2^2 \leq \lambda_{\max}(P) \left\|\frac{\partial \bar{x}(0)}{\partial \theta_i}\right\|_2^2 + \frac{1}{4\,|\mu|^3} \left\|\frac{\partial \bar{A}}{\partial \theta_i}\right\|_2^2 \left\|\bar{C}^T\bar{C}\right\|_2 \|\bar{x}(0)\|_2^2 + \frac{1}{2\,|\mu|^2} \left\|\frac{\partial \bar{A}}{\partial \theta_i}\right\|_2 \left\|\bar{C}^T\bar{C}\right\|_2 \|\bar{x}(0)\|_2 \left\|\frac{\partial \bar{x}(0)}{\partial \theta_i}\right\|_2 \quad (15)$$

*where $P$ is the Lyapunov matrix and $\mu$ depends on $\bar{A}$ as in Lemma 1.*

*Proof.* The proof follows by using the product rule for the derivative of $\zeta(t,\theta)$ in equation (7) along with the results from Theorem 1 and 2. □

### C. Nonlinear Dynamics

For nonlinear system dynamics, the approach above to derive the bound on the robustness guarantee does not work because we cannot obtain the error dynamics analytically as was possible for linear dynamics in equation (7). An alternate approach for deriving a bound on the sensitivity of the error is using local sensitivity analysis. We used this method in our previous work [26] to derive the robustness estimates. We will briefly summarize the results using the sensitivity analysis approach for nonlinear dynamics in this section and then show that for linear systems it results in an equivalent bound as obtained in the previous section. Consider the following nonlinear dynamics of the full system

$$\dot{x} = f(x,\Theta), \quad y = Cx, \quad x(0) = x_0. \quad (16)$$

The reduced nonlinear model is given using similar notation

$$\dot{\hat{x}} = \hat{f}(\hat{x},\Theta), \quad \hat{y} = \hat{C}\hat{x}, \quad \hat{x}(0) = \hat{x}_0. \quad (17)$$

Similar to the linear case, we assume that both the full model and the reduced model are asymptotically stable. Note that although we have a linear output-state relationship, the results that we will show can be extended to the general case of nonlinear output-state equation as well. We derived these extension results in [34].

**Theorem 3.** *For the structured model reduction of the nonlinear dynamical system (16) to the reduced system (17) by using time-scale separation and quasi-steady state approximation, the norm of the sensitivity of the error in model reduction, $S_\zeta$ is bounded above by*

$$\|S_\zeta\|_2^2 \leq \lambda_{\max_{\bar{x}}}(P(\bar{x})) \left\|\bar{S}(0)\right\|_2^2 + 2\int_0^\infty \left\|\bar{Z}^T P(\bar{x})\bar{S}\right\|_2 dt + \lambda_{\max_{\bar{x}}}(\dot{P}(\bar{x})) \int_0^\infty \left\|\bar{S}\right\|_2^2 dt \quad (18)$$

*where $P(\bar{x})$ is a matrix that solves the Lyapunov equation $\bar{J}(\bar{x})^T P(\bar{x}) + P(\bar{x})\bar{J}(\bar{x}) = -\bar{C}^T\bar{C}$, $\bar{J}(\bar{x})$ is the Jacobian matrix at point $\bar{x}$, $\bar{Z}$ is the sensitivity to parameter and $\bar{S}$ is the sensitivity coefficients vector of the augmented system, given by:*

$$\bar{J}(\bar{x}) = \begin{bmatrix} \frac{\partial f}{\partial x} & 0 \\ 0 & \frac{\partial \hat{f}}{\partial \hat{x}} \end{bmatrix}, \quad \bar{Z} = \begin{bmatrix} \frac{\partial f}{\partial \theta_i} \\ \frac{\partial \hat{f}}{\partial \theta_i} \end{bmatrix}, \quad \bar{S} = \begin{bmatrix} \frac{\partial x}{\partial \theta_i} \\ \frac{\partial \hat{x}}{\partial \theta_i} \end{bmatrix}.$$

*Proof Sketch.* We will only sketch the proof here for completeness, the full proof is given in [26]. Write the sensitivity system equations [32] for the augmented nonlinear dynamical system at the point $\bar{x}(t) = \bar{x}$:

$$\dot{\bar{S}} = \bar{J}(\bar{x})\bar{S} + \bar{Z}$$

where $\bar{S}, \bar{J}(\bar{x})$, and $\bar{Z}$ are as defined in the theorem. Then, the sensitivity of the error is given by $S_\zeta = \bar{C}\bar{S}$. With this setup, it is straightforward to compute the bound by writing down the 2-norm definition for $S_\zeta$ and then using the time-derivative of a Lyapunov function ($V(\bar{S}) = \bar{S}^T P(\bar{x})\bar{S}$) to substitute for $\bar{S}^T\bar{C}^T\bar{C}\bar{S}$ using the Lyapunov equation in the resulting integral. □

Note that to use the above result to give a robustness guarantee bound for a model reduction, we need to compute all local sensitivity coefficients. However, the bound obtained in the linear case was a much simpler computation as it only involved the computation of the sensitivity of $\bar{A}$ and the initial conditions $\bar{x}(0)$ to the parameters. We will show next that the final bound for both methods is the same in the case of linear dynamics.

### D. Equivalence of the two results for linear dynamics

A direct comparison of the results in Corollary 2.1 and Theorem 3 is not evident. But for the special case of linear dynamics, we have closed-form solutions for $\bar{S}(t)$ and hence $\bar{Z}(t)$. For linear dynamics, we can write the result in Theorem 3 as

$$\begin{aligned} \|S_\zeta\|_2^2 &\le \lambda_{\max}(P) \left\|\bar{S}(0)\right\|_2^2 \\ &\quad + 2\int_0^\infty \left\| \left(\frac{\partial \bar{A}}{\partial \theta_i}\bar{x}\right)^T P\bar{S}\right\|_2 dt. \end{aligned} \tag{19}$$

Note that here we have, $\bar{J} = \bar{A}$.

*Claim.* The bound on the sensitivity of the error in model reduction when obtained using sensitivity analysis approach (as in equation (19)) is same as the bound obtained using direct linear analysis approach (as in equation (15)). In particular, we have that,

$$\begin{aligned} 2\int_0^\infty \left\| \left(\frac{\partial \bar{A}}{\partial \theta_i}\bar{x}\right)^T P\bar{S}\right\| dt &= \frac{1}{4\,|\mu|^3}\left\|\frac{\partial \bar{A}}{\partial \theta_i}\right\|^2 \left\|\bar{C}^T\bar{C}\right\| \left\|\bar{x}(0)\right\|^2 \\ &+ \frac{1}{2\,|\mu|^2}\left\|\frac{\partial \bar{A}}{\partial \theta_i}\right\| \left\|\bar{C}^T\bar{C}\right\| \left\|\bar{x}(0)\right\| \left\|\frac{\partial \bar{x}(0)}{\partial \theta_i}\right\| \end{aligned} \tag{20}$$

Note that the first term in equations (15) and (19) is the same and hence we have removed that term in the equation above. This term corresponds to the parametric uncertainty in the initial conditions.

*Proof.* To prove the above claim, we start by evaluating the different parts of the left hand side expression using the closed-form solutions for linear dynamics. First, note that from the sensitivity equation [32] for linear system we have that

$$\dot{\bar{S}} = \bar{A}\bar{S} + \frac{\partial \bar{A}}{\partial \theta_i}\bar{x}(t). \tag{21}$$

Solving the equation above for $\bar{S}(t)$ and taking the norm we get

$$\begin{aligned} \left\|\bar{S}(t)\right\| &\le \left\|e^{\bar{A}t}\bar{S}(0)\right\| + \left\|\int_0^t e^{\bar{A}(t-\tau)}\frac{\partial \bar{A}}{\partial \theta_i}\bar{x}(\tau)d\tau\right\| \\ &\le e^{-|\mu|t}\left\|\bar{S}(0)\right\| + \left\|\frac{\partial \bar{A}}{\partial \theta_i}\right\| \left\|\bar{x}(0)\right\| te^{-|\mu|t}. \end{aligned} \tag{22}$$

using Lemma 1 and 2. Similarly, for $\left\|\bar{Z}\right\|$, we have

$$\left\|\bar{Z}\right\| = \left\|\frac{\partial \bar{A}}{\partial \theta_i}\bar{x}\right\| \le \left\|\frac{\partial \bar{A}}{\partial \theta_i}\right\| \left\|\bar{x}(0)\right\| e^{-|\mu|t}. \tag{23}$$

Finally, for the Lyapunov matrix, we know that

$$\|P\| = \left\|\int_0^\infty e^{\bar{A}^T t}\bar{C}^T\bar{C}e^{\bar{A}t}dt\right\|,$$

using the observability Gramian. Using Lemma 1, we have

$$\|P\| \le \int_0^\infty e^{-|\mu|t}\left\|\bar{C}^T\bar{C}\right\| e^{-|\mu|t}dt.$$

So,

$$\|P\| \le \left\|\bar{C}^T\bar{C}\right\| \int_0^\infty e^{-2|\mu|t}dt \Rightarrow \|P\| \le \frac{1}{2\,|\mu|}\left\|\bar{C}^T\bar{C}\right\|. \tag{24}$$

Substituting the equations (22), (23), and (24) into the left hand size of equation (20), we get the desired result that proves our claim. □

Although the two approaches give equivalent results for linear dynamics, the advantage with the sensitivity analysis approach is that it is a general method that can be used for nonlinear dynamical systems as well.

## IV. Examples

In this section, we demonstrate the computation of robustness guarantees using examples from biomolecular systems. First, consider an enzymatic reaction system that has two chemical reactions: $E + S \underset{d}{\overset{a}{\rightleftharpoons}} C$, $C \xrightarrow{k} E + P$ to model the binding of an enzyme $E$ to a substrate $S$ forming a complex $C$ that then catalyzes to form the product $P$. It is well-known [35] that singular perturbation theory can be used to derive a reduced-order model for this system. Since for all biologically relevant parameter values, this system does not become unstable, we may not be able to use the singular perturbation margin to estimate robustness of this model reduction [36]. However, our method is still applicable as it depends on computing the sensitivity of the system states to the parameters. Further, as our second example, we consider a chemical reaction network (CRN) model of gene expression [37] — a gene (G) gets transcribed by RNA polymerase (P) to form mRNA (T) that is then translated by ribosomes (R) to express a protein (X). For the CRN, we have that P binds to T reversibly with reaction rates $k_{bp}$ and $k_{up}$ for binding and unbinding respectively. Similarly, we have $k_{br}$ and $k_{ur}$ for the binding of R to T. The transcription and translation rates are $k_{tx}$ and $k_{tl}$ while the degradation parameters for $T$ and $X$ are given by $d_T$ and $d_X$ respectively. For this CRN model, it is not possible to derive reduced models using singular perturbation theory since it is not clear how we could transform the system dynamics to the standard form (as in equation (3)). We may use QSSA to derive accurate reduced models in certain parameter regimes as shown in [38]. In particular, we consider the reduced model with the mRNA and protein dynamics (see Appendix B for more details). To demonstrate the robustness estimate computations in the linear case, we linearize the full and the reduced model dynamics at all points of interest in the state-space. The robustness bound on $\|S_\zeta\|$ for each parameter with time is shown in Figure 2. As discussed earlier, an alternative approach is to use the result in Theorem 3 to derive bounds directly for the nonlinear systems. With this method, we get a time-integrated result for $\|S_\zeta\|$, which is of the order of $10^4$ whereas we see in Figure 2 that the bound on $\|S_\zeta\|$ with the linearization approach is of the order of $10^2$. Hence, the linear analysis approach (from Theorem 2) gives less conservative results than the direct nonlinear approach (from Theorem 3) but requires the linearization approximation at every point in the system trajectory so it may not always be accurate and feasible. The results for all examples and the corresponding Python code to reproduce the figures is available to run online [39].

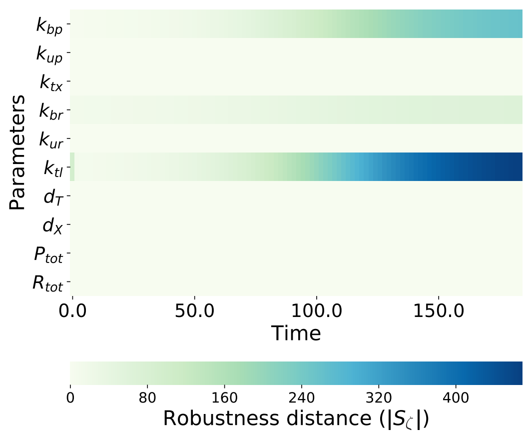


Fig. 2. Robustness estimates using the result given in Theorem 2 for a gene expression system. Observe that the model reduction error $\zeta$ is most sensitive to the translation parameter $k_{tl}$. This observation is consistent with the result obtained using the nonlinear approach [38, Fig.2].

## V. Conclusions

Our main result gives a closed-form expression for the robustness guarantee of structured model reduction of linear dynamical systems. We show two different methods to derive this result — a direct linear analysis approach for the linear systems and a sensitivity analysis based approach that also works for nonlinear dynamics. We also show that the two methods are equivalent for linear systems. Although robustness guarantee metrics do not exist for general structured model reduction, there are results for robustness analysis of singular perturbation based model reduction. Since singularly perturbed systems are a special case of the problem formulation in this paper, we compared the results of our method with a robustness analysis method for singularly perturbed systems. The advantage of our method is that the system does not need to be in the standard form as in singular perturbation theory and that we can compute the robustness of the model reduction error with respect to each model parameter individually for a holistic analysis of different possible model reductions. An interesting future line of work could be to study the relationship between our robustness analysis method and other conventional methods in robust control theory.


## Acknowledgment

We would like to thank the reviewers for their insightful comments. The author A.P. would like to acknowledge funding support from NSF grant CBET-1903477.


## References


[1] P. Kokotović, H. K. Khalil, and J. O'reilly, *Singular perturbation methods in control: analysis and design*. SIAM, 1999.

[2] S. Z. Rizvi, J. Mohammadpour, R. Tóth, and N. Meskin, "A kernel-based pca approach to model reduction of linear parameter-varying systems," *IEEE Transactions on Control Systems Technology*, vol. 24, no. 5, pp. 1883–1891, 2016.

[3] B. Moore, "Principal component analysis in linear systems: Controllability, observability, and model reduction," *IEEE Transactions on Automatic Control*, vol. 26, no. 1, pp. 17–32, 1981.

[4] M. K. Transtrum and P. Qiu, "Bridging mechanistic and phenomenological models of complex biological systems," *PLoS computational biology*, vol. 12, no. 5, p. e1004915, 2016.

[5] S. Rao, A. Van der Schaft, K. Van Eunen, B. M. Bakker, and B. Jayawardhana, "A model reduction method for biochemical reaction networks," *BMC systems biology*, vol. 8, no. 1, pp. 1–17, 2014.

[6] H. Sandberg and R. M. Murray, "Model reduction of interconnected linear systems," *Optimal Control Applications and Methods*, vol. 30, no. 3, pp. 225–245, 2009.

[7] A. Sootla and J. Anderson, "On projection-based model reduction of biochemical networks part i: The deterministic case," in *53rd IEEE Conference on Decision and Control*. IEEE, 2014, pp. 3615–3620.

[8] A. Gorban, "Model reduction in chemical dynamics: slow invariant manifolds, singular perturbations, thermodynamic estimates, and analysis of reaction graph," *Current Opinion in Chemical Engineering*, vol. 21, pp. 48–59, 2018.

[9] P. Kokotovic and P. Sannuti, "Singular perturbation method for reducing the model order in optimal control design," *IEEE Transactions on Automatic Control*, vol. 13, no. 4, pp. 377–384, 1968.

[10] R. Marino and S. Nicosia, "Singular perturbation techniques in the adaptive control of elastic robots," *IFAC Proceedings Volumes*, vol. 18, no. 16, pp. 95–100, 1985.

[11] K. R. Schneider and T. Wilhelm, "Model reduction by extended quasi-steady-state approximation," *Journal of Mathematical Biology*, vol. 40, no. 5, pp. 443–450, 2000.

[12] N. Vora and P. Daoutidis, "Nonlinear model reduction of chemical reaction systems," *AIChE Journal*, vol. 47, no. 10, pp. 2320–2332, 2001.

[13] F. G. Helfferich, "Systematic approach to elucidation of multistep reaction networks," *The Journal of Physical Chemistry*, vol. 93, no. 18, pp. 6676–6681, 1989.

[14] J. A. Christiansen, "The elucidation of reaction mechanisms by the method of intermediates in quasi-stationary concentrations," in *Advances in Catalysis*. Elsevier, 1953, vol. 5, pp. 311–353.

[15] T. Turanyi, A. Tomlin, and M. Pilling, "On the error of the quasi-steady-state approximation," *The Journal of Physical Chemistry*, vol. 97, no. 1, pp. 163–172, 1993.

[16] A. Yannacopoulos, A. Tomlin, J. Brindley, J. Merkin, and M. Pilling, "The error of the quasi steady-state approximation in spatially distributed systems," *Chemical Physics Letters*, vol. 248, no. 1-2, pp. 63–70, 1996.

[17] A. Papachristodoulou, Y.-C. Chang, E. August, and J. Anderson, "Structured model reduction for dynamical networked systems," in *49th IEEE Conference on Decision and Control (CDC)*. IEEE, 2010, pp. 2670–2675.

[18] R. Babaghasabha, M. A. Khosravi, and H. D. Taghirad, "Adaptive robust control of fully constrained cable robots: singular perturbation approach," *Nonlinear Dynamics*, vol. 85, no. 1, pp. 607–620, 2016.

[19] L. A. Belhaj, M. Ait-Ahmed, and M. F. Benkhoris, "Embarked electrical network robust control based on singular perturbation model," *ISA transactions*, vol. 53, no. 4, pp. 1143–1151, 2014.

[20] J. C. Doyle, B. A. Francis, and A. R. Tannenbaum, *Feedback Control Theory*. Dover, 2009.

[21] M. K. Fan, A. L. Tits, and J. C. Doyle, "Robustness in the presence of joint parametric uncertainty and unmodeled dynamics," in *1988 American control conference*. IEEE, 1988, pp. 1195–1200.

[22] J. Freudenberg, D. Looze, and J. Cruz, "Robustness analysis using singular value sensitivities," *International Journal of Control*, vol. 35, no. 1, pp. 95–116, 1982.

[23] X. Yang, J. J. Zhu, and A. S. Hodel, "Singular perturbation margin and generalised gain margin for linear time-invariant systems," *International Journal of Control*, vol. 88, no. 1, pp. 11–29, 2015.

[24] X. Yang and J. J. Zhu, "Singular perturbation margin and generalised gain margin for nonlinear time-invariant systems," *International Journal of Control*, vol. 89, no. 3, pp. 451–468, 2016.

[25] H. K. Khalil and J. W. Grizzle, *Nonlinear Systems*. Prentice Hall, Upper Saddle River, NJ, 2002, vol. 3.

[26] A. Pandey and R. M. Murray, "An automated model reduction tool to guide the design and analysis of synthetic biological circuits," *bioRxiv*, p. 640276, 2019.

[27] J. Schmidt, "G. dahlquist, stability and error bounds in the numerical integration of ordinary differential equations. 85 s. stockholm 1959. k. tekniska högskolans handlingar," 1961.

[28] T. Ström, "On logarithmic norms," *SIAM Journal on Numerical Analysis*, vol. 12, no. 5, pp. 741–753, 1975.

[29] R. F. Snider, "Perturbation variation methods for a quantum boltzmann equation," *Journal of Mathematical Physics*, vol. 5, no. 11, pp. 1580–1587, 1964.

[30] R. M. Wilcox, "Exponential operators and parameter differentiation in quantum physics," *Journal of Mathematical Physics*, vol. 8, no. 4, pp. 962–982, 1967.

[31] H. Tsai, K. Chan *et al.*, "A note on parameter differentiation of matrix exponentials, with applications to continuous-time modelling," *Bernoulli*, vol. 9, no. 5, pp. 895–919, 2003.

[32] R. P. Dickinson and R. J. Gelinas, "Sensitivity analysis of ordinary differential equation systems - a direct method," *Journal of Computational Physics*, vol. 21, no. 2, pp. 123–143, 1976.

[33] P. J. Antsaklis and A. N. Michel, *Linear Systems*. Springer Science & Business Media, 2006.

[34] A. Pandey and R. M. Murray, "Model reduction tools for phenomenological modeling of input-controlled biological circuits," *bioRxiv*, 2020.

[35] D. Del Vecchio and R. M. Murray, *Biomolecular Feedback Systems*. Princeton University Press Princeton, NJ, 2015.

[36] X. Yang and J. J. Zhu, "Singular perturbation margin assessment of linear time-invariant systems via the bauer-fike theorems," in *2012 IEEE 51st IEEE Conference on Decision and Control (CDC)*. IEEE, 2012, pp. 6521–6528.

[37] W. Poole, A. Pandey, Z. Tuza, A. Shur, and R. M. Murray, "Biocrnpyler: Compiling chemical reaction networks from biomolecular parts in diverse contexts," *BioRxiv*, 2020.

[38] A. Pandey and R. M. Murray, "A two-state ribosome and protein model can robustly capture the chemical reaction dynamics of gene expression," *bioRxiv*, 2020.

[39] A. Pandey, "Python notebook for model reduction robustness estimates," *Google Colaboratory*, 2021, [Online].

[40] ——, "Auto-reduce : Python based automated model reduction package," *GitHub*, 2021, [Online].


## Appendix A

*Proof of equation (8) in Lemma 2.* For a linear system, $\dot{x} = Ax$, we can write the solution $x(t) = e^{At}x(0)$, where $e^{At}$ is the matrix exponential. Now, for a parameter $\theta_i$, we can write

$$\frac{\partial x(t)}{\partial \theta_i} = e^{At}\frac{\partial x(0)}{\partial \theta_i} + \frac{\partial e^{At}}{\partial \theta_i}x(0),$$

using the product rule of differentiation. Define

$$S(t) := \frac{\partial x(t)}{\partial \theta_i}, \tag{25}$$

so we have,

$$S(t) = e^{At}S(0) + \frac{\partial e^{At}}{\partial \theta_i}x(0), \tag{26}$$

and write $\dot{S}(t)$ using equation (25) and $\dot{x} = Ax$ as

$$\frac{dS}{dt} = A\frac{\partial x}{\partial \theta_i} + \frac{\partial A}{\partial \theta_i}x = AS + \frac{\partial A}{\partial \theta_i}x.$$

Solving for $S(t)$, we get,

$$S(t) = e^{At}S(0) + \int_o^t e^{A(t-\tau)}\frac{\partial A}{\partial \theta_i}x(\tau)d\tau.$$

Since $x(\tau) = e^{A\tau}x(0)$, we can simplify the above equation and write

$$S(t) = e^{At}S(0) + \left[\int_o^t e^{A(t-\tau)}\frac{\partial A}{\partial \theta_i}e^{A\tau}d\tau\right]x(0).$$

Comparing this with equation (26), we get the desired result for the derivative of the matrix exponential

$$\frac{\partial e^{At}}{\partial \theta_i} = \int_o^t e^{A(t-\tau)}\frac{\partial A}{\partial \theta_i}e^{A\tau}d\tau. \qquad \square$$

## Appendix B

Using mass-action kinetics for the CRN described in Section IV and conservation laws with fixed total RNA polymerase ($P_{\text{tot}}$) and total ribosome ($R_{\text{tot}}$) we get the following nonlinear system dynamics [38]:

$$\begin{aligned}
\frac{dP}{dt} &= (k_{tx} + k_{up})(P_{\text{tot}} - P) - k_{bp}GP,\\
\frac{dT}{dt} &= k_{tx}(P_{\text{tot}} - P) + (k_{tl} + k_{ur})(R_{\text{tot}} - R) - k_{br}RT - d_T T,\\
\frac{dR}{dt} &= (k_{tl} + k_{ur})(R_{\text{tot}} - R) - k_{br}RT,\\
\frac{dX}{dt} &= k_{tl}(R_{\text{tot}} - R) - d_X X.
\end{aligned}$$

For this full system dynamics, we can derive various reduced-order models. In this paper, we consider the reduced model with the mRNA and protein dynamics. This reduced model is obtained by setting all other states to be at QSSA (using the AutoReduce [40] package):

$$\begin{aligned}
\frac{d\hat{T}}{dt} &= k_{tx}P_{\text{tot}}\frac{G}{\frac{k_{tx}+k_{up}}{k_{bp}} + G} - d_T\hat{T}\\
\frac{d\hat{X}}{dt} &= k_{tl}R_{\text{tot}}\frac{\hat{T}}{\frac{k_{tl}+k_{ur}}{k_{br}} + \hat{T}} - d_X\hat{X},
\end{aligned}$$

where $\hat{T}$ and $\hat{X}$ represent the reduced states for mRNA T and protein X. We can obtain linearized dynamics at every point in the system trajectory. So for a point $x^* = [P^*, T^*, R^*, X^*]$, we have the following system matrices:

$$A = \begin{bmatrix} -Gk_{bp} - k_{tx} - k_{up} & 0 & 0 & 0 \\ -k_{tx} & -k_{br}R^* - d_T & -k_{br}T^* - k_{tl} - k_{ur} & 0 \\ 0 & -k_{br}R^* & -k_{br}T^* - k_{tl} - k_{ur} & 0 \\ 0 & 0 & -k_{tl} & -d_X \end{bmatrix},$$

$$\hat{A} = \begin{bmatrix} -d_T & 0 \\ \frac{R_{\text{tot}}k_{tl}}{T^* + \frac{k_{tl}+k_{ur}}{k_{br}}} & -d_X \end{bmatrix}.$$

We can then derive $\frac{\partial A}{\partial \theta_i}$ for each parameter $\theta_i \in \theta$ to compute the robustness estimate bounds for this system using the result in Theorem 2.